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ANNUAL TECHNICAL REPORT

AFOSR-90-0143

December 1990

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The objective of this research program is to identify relationships between characteristics of intermetallic alloys at an atomic scale, the operation of slip and twinning deformation mechanisms at a microstructural scale, and bulk deformation and fracture properties. Our research focuses on two fundamental aspects of the problem of low toughness of intermetallic alloys: The role of deformation twinning in promoting ductility and toughness of ordered intermetallic alloys, and modeling the effect of dislocation characteristics on crack tip plasticity.

Part I: Progress

In Part I we seek to establish the role of deformation twinning in promoting ductile behavior in intermetallic alloys, and to identify how twinning is influenced by characteristics of the ordered structure. We have selected, for this study, Al_3Nb alloys with additions of various transition elements. Five different compositions have been prepared to date: 75at.%Al-35at.%Nb; 75 at.%Al-23.75at.%Nb-1.25at.%Ti; 75at.%Al-22.5at.%Nb-2.5at.%Ti; 75at.%Al-20at.%Nb-5at.%Ti; 75at.%Al-12.5at.%Nb-12.5at.%Ti. The alloys were prepared using elemental powders of aluminum, niobium and titanium by a solid/liquid reaction synthesis. The elemental powders were blended together in the appropriate stoichiometric ratios, canned, degassed, sealed in vacuum, heated to melt the aluminum and to complete the reaction, and finally HIPed under argon to fully densify the reaction product. Light metallography revealed a very fine, uniform grain structure. However, in some cases a discrete cell-like structure, believed to be a second phase, was obtained.

X-ray diffraction analysis indicated that the major phase, in excess of 95 volume percent, for all alloy compositions was Al_3Nb. Weak diffraction lines from other phases were also detected and the intensity of these extraneous diffraction lines increased with titanium content. This observation is consistent with the light metallographic examination which also revealed that the percentage of second phase increased with titanium content. We have not identified the structure of the second phase at this time.

However, these results indicate that the substitution for Nb by Ti may not be very high, i.e. probably less than 20%.

We have identified some problems associated with sample preparation which we are attempting to correct. Using SEM and EDS we have concluded that we have a contamination of Fe, Ni, and Cr in our final product. These impurities are from the stainless steel tube that was employed for the synthesis at 900°C and is associated with the liquid/solid reaction. We are now attempting to prepare samples by arc-melting prior to using the HIP.

The long-range order parameter is being determined as a function of temperature for the various alloy compositions. In addition we are measuring the hardness of the samples as a function of temperature and will be examining the deformation behavior adjacent to the hardness measurements. The major problems we have encounted thus far have been associated with sample preparation. However, we believe that we have identified all of the problems and have developed processing methods to eliminate them. A sufficient quantity of high purity samples should be available by the end of the year to allow us to focus on the main objective of this research, i.e. to establish atomic structure/deformation relationships.

Part II: Progress

Low toughness is one of the principal factors preventing use of ordered intermetallic alloys as engineering materials. Some ordered intermetallic alloys have low toughness as a consequence of grain boundary fracture caused by poor grain boundary cohesion or by segregation of impurities to grain boundaries. Other ordered intermetallic alloys with low toughness exhibit transgranular cleavage fracture prior to general yielding. Traditionally, cleavage fracture has been associated with high-strength materials (such as ceramics) in which crack tip plasticity is limited by the high yield strength. However, many ordered intermetallic alloys which exhibit cleavage fracture have low or moderate strength. The goal of Part II of the present research project is to model the behavior of dislocations in the crack tip region in several ordered intermetallic alloys to identify the cause of cleavage fracture in these materials.

In most materials, toughness results from crack tip plasticity which reduces the high stress concentration at the crack tip. Rice and Thomson [Phil. Mag., **29** (1974) 73] proposed that an energy barrier can prevent dislocations from being emitted from crack tips in some materials, thereby inhibiting crack tip plasticity. The energy barrier is formed as a result of the interaction of a dislocation with the stress field near the crack tip and with the free surface of the crack, but it does not depend on the yield strength of the material. The Rice-Thomson model has been tested for a wide variety of materials and excellent correlation has been found between the model results and the experimentally-observed fracture mode.

A variety of ordered intermetallic alloys exhibit the combination of low toughness and low or modest strength that is difficult to explain based on traditional fracture concepts. It is possible that an energy barrier to dislocation emission from crack tips is the cause of low toughness in these materials. However, modeling of dislocation emission from crack tips in ordered intermetallic alloys requires modeling the complex dissociated superlattice dislocation configurations that occur in these materials. During the first part of the present research project, a model for dislocation emission from crack tips in ordered intermetallic alloys with the $L1_2$ crystal structure has been formulated. The model involves numerical calculation of dislocation energy as a function of position near a crack tip. The model was formulated to simulate emission of perfect superlattice dislocations, APB-coupled partial superlattice dislocation pairs, and SISF-coupled partial superlattice dislocation pairs. The model inputs are 5 material properties and 2 geometrical characteristics of the slip system. The principal result is the activation energy for emission of the various types of dislocations from a crack tip in an $L1_2$ crystal.

The model results have been correlated with experimentally-observed fracture modes for 7 ordered intermetallic alloys with the $L1_2$ crystal structure. This comparison has led to definition of a parameter (f) that describes the range of slip system orientations for which there is no energy barrier to dislocation emission from a crack tip. The results indicate that a critical value of f is required for a material to be ductile or tough on a macroscopic scale. Alloys with values of f below the critical value are not tough because crack tip plasticity cannot occur in a sufficient number of grains.

In addition to accounting for low toughness in several ordered intermetallic alloys with the $L1_2$ crystal structure, the model has been used to predict changes in material properties that could increase the toughness. The family of $L1_2$ intermetallic alloys with composition $(Al,X)_3Ti$ (X = Ni, Fe, Cu, Pd, Cr, Mn) have attractive physical, mechanical and environmental properties, except for extremely poor room temperature toughness. Modeling results indicate that lowering the APB or SISF energy of one of these alloys to a value below about 150 mJ/m^2 would be sufficient to permit extensive crack tip plasticity. Unless other brittle fracture modes intervene (such as grain boundary fracture) this would have the desirable result of increasing the macroscopic toughness of the alloy. It is not known what alloying elements could achieve this reduction of APB or SISF energy, but several researchers in the US are investigating this family of alloys and we have discussed the modeling results with them. A paper is in preparation describing the results of this phase of the investigation and the results will be presented at the TMS meeting in February 1991 in New Orleans.

Modeling of dislocation behavior in the vicinity of crack tips in ordered intermetallic alloys with the $L1_2$ crystal structure is nearly complete. Based on the excellent correlation between modeling results and experimental observations, it is appropriate to extend the model to ordered intermetallic alloys with other crystal structures. It is our intention to model dislocation emission from crack tips in alloys with the B2 crystal structure (for example: NiAl). Future work may also include experimental evaluation to test model predictions and evaluation of the effect of deformation twinning on crack tip plasticity and toughness of ordered intermetallic alloys.

List of Publications and Presentations

AFOSR-90-0143
1990

Publication

In preparation

M.F. Bartholomeusz and J.A. Wert, "Effect of Dislocation Dissociation on Crack Tip Plasticity in $L1_2$ Ordered Intermetallic Alloys," to be submitted to Journal of Materials Research.

Presentation

J.A. Wert, "Microstructure, Deformation and Fracture of $Al_{67}Ni_8Ti_{25}$ and Similar $(Al,X)_3Ti$ Intermetallic Alloys," General Dynamics Corp., Fort Worth, August 21, 1990.

List of Publications and Presentations

AFOSR-87-0082-A
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Publications

H. Gudmundsson, D. Brooks and J.A. Wert, "Mechanisms of Continuous Recrystallization in an Al-Zr-Si Alloys," accepted for publication in Acta Metallurgica et Materialia.

D.D. Brooks, H. Gudmundsson, and J.A. Wert, "Continuous Recrystallization in an Al-Zr-Si Alloy and an Al-Cu-Zr-Si Alloys," to be published in Hot Deformation of Aluminum Alloys.

C.P. Blankenship, Jr., and E.A. Starke, Jr., "The Fatigue Crack Growth Behavior of the Al-Cu-Li Alloy Weldalite 049," Fatigue & Fracture of Engineering Materials and Structures 14, 103-114 (1990).

W.E. Quist and E.A. Starke, Jr., "The Microstructure and Properties of Aluminum-Lithium Alloys," New Light Alloys, AGARD Lecture Series No. 174, AGARD, Neuilly Sur Seine, France, 2-1 - 2-21 (1990).

Presentation

E.A. Starke, Jr. (with W. Quist), "The Microstructure and Properties of Al-Li Alloys," AGARD/NATO New Light Alloys Lecture, Spain, France, and Monterey, USA, October 1990.